

Application of externally-coupled BES-CFD in HAM engineering of the indoor environment

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APPLICATION OF EXTERNALLY-COUPLED BES-CFD IN HAM ENGINEERING OF THE INDOOR ENVIRONMENT

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ABSTRACT

The high importance of indoor environment performance aspects such as surface condensation, mold growth, thermal comfort, etc., is widely recognized. High-resolution simulation of heat, air and moisture (HAM) transfer can be used to enhance the prediction and analysis of these aspects. For this purpose, a coupling mechanism has been developed in order to perform run-time external coupling between Building Energy simulation (BES) and Computational Fluid Dynamics (CFD). This paper presents the results of indoor humidity calculation using the new coupled tool for the BESTEST case-600. The results are compared with stand-alone BES results and the need and importance of coupled simulations is discussed.

INTRODUCTION

Several Building Performance Simulation (BPS) tools exist to study HAM transfer in the built environment. They are characterized by a large variation in modelling level and spatial and temporal resolution. Building Energy Simulation (BES) tools can be used for the simulation of HAM transfer for an entire year. These are powerful tools, but generally include simplified airflow, heat and moisture transfer modelling. For example, surface transfer coefficients are often incorporated in a simplified way by fixed values or empirical correlations and heat and mass transfer analogies. Detailed HAM modelling of the building interior is possible with Computational Fluid Dynamics (CFD). However, the implementation of meteorological boundary conditions and the capabilities for efficient transient modelling are significantly less advanced than in BES tools.

Integration of BES tools with CFD by using internal coupling has been investigated for indoor air climate with different degrees of complexity (Negrao, 1995; Zhai, 2003; Beausoleil-Morrison, 2000). In this approach, a CFD module is developed within a BES environment. Due to this coupling approach, the final numerical package, which is one single package, might suffer from certain limitations in the long term. Developing and maintaining one single package to include all physical domains (heat, air and moisture) is expensive and includes: the background research,

development of a pilot program, validation of the program, implementation trials, improvement of the software and documentation and then the commercial exploitation (Maver & Ellis, 1982). On the other hand, one may encounter a certain amount of limitations and deficiencies such as lack of some features and options when working with a single package.

A solution which has been adopted recently is run-time external coupling of distributed applications. By this approach the existing numerical packages for specific geometrical or physical domains work together and exchange data at predefined or calculated time-steps. It has been recognized and justified that the final distributed simulation environment is more flexible, practical, and powerful than the sum of the individual software programs (Trcka et al., 2006).

In the past, efforts have been made to perform high-resolution simulation for the indoor environment via run-time external coupling of BES (ESP-r) and CFD (FLUENT) (Djunaedy, 2005). Previous work on this integration included heat and air as the physical domains. In other words, convective heat transfer coefficients (h_c) and surface temperatures were exchanged between CFD and BES.

This paper presents a coupled BES-CFD approach that includes an additional physical domain: moisture. In this study, the moisture balance equation in ESP-r is connected to FLUENT via convective moisture transfer coefficients (h_m) and surface humidity ratios. ESP-r and FLUENT run in parallel and exchange data on a time-step basis.

This paper consists of two main parts. The first part starts by describing the well-mixed zonal model for moisture, which is implemented in ESP-r and in many other BES tools. Then it introduces the effective moisture penetration depth (EMPD) model and discusses the necessity of its implementation for BES-CFD coupling. In the second part of the paper, the newly developed BES-CFD prototype (briefly referred to as "prototype" in this paper), is introduced. In this part, first the capabilities and deficiencies of BES and CFD tools are discussed. Then it presents the interface variables and their coupling requirements. Different coupling strategies are explained and the first results of an externally

coupled BES-CFD simulation using loose coupling are presented for the BESTEST case 600.

MOISTURE BALANCE EQUATION

BES tools assume perfect mixing of indoor air and therefore a single node represents the entire air volume. The moisture balance equation for the air node can be given by:

$$\frac{V}{R_v T} \frac{dp}{dt} = g_{\text{equ/peo}} + g_{\text{ven/inf}} + g_{\text{cond}} +$$

$$g_{\text{sys}} + g_{\text{source/sink}} + g_{\text{constr}}$$

(the nomenclature is presented at the end of the paper).

The left hand side of Eq (1) describes the rate of change in vapour pressure for the air node. The right hand side represents, respectively, the moisture gains from equipment and occupants, moisture added or removed by ventilation and infiltration, moisture condensation, moisture gains related to the HVAC system, moisture added or removed by other sources and sinks and finally moisture adsorbed or desorbed by the building envelope. The last term in the equation is given by the following expression:

$$g_{\text{constr}} = \sum_{i=1}^n A_i h_{m,i} (p_{s,i} - p_r) \quad (2)$$

which is the moisture flux from the wall surfaces into indoor environment. The moderating influence of hygroscopic building materials on the indoor relative humidity and its significant importance for indoor air quality has been investigated by many researchers in the past (Gulick, 1911; Ingersoll, 1913; Menzies, 1913; Padfield, 1999; Svennberg et al., 2007; Janssen & Roels, 2008). In order to model the water vapour flux to the indoor environment, different numerical approaches can be applied. The building envelope HAM model, which is already implemented in ESP-r (Nakhi, 1995), is an option. Nevertheless, this part of the ESP-r source code has not been kept updated for a long time, which has led to inconsistencies between the present version of ESP-r and this HAM model. Therefore, the use of this module in ESP-r was not possible for the authors. The second option would be co-simulation of ESP-r with other building envelope HAM models such as HAMFEM (Janssen, 2002; Janssen et al., 2007), WUFI (Künzel, 1994; Künzel et al., 2004), CHAMPS (Grunewald, 1997; Grunewald & Nicolai, 2006) etc. This option is currently being pursued (Costola et al., 2008), and the final results will be available in the near future. Considering those options, it was decided to implement, for now, the effective moisture penetration depth (EMPD) model (Kerestecioglu et al., 1990) in ESP-r. The EMPD model as a moisture inertia model (which means it takes into account the damping effect of hygroscopic materials on the relative humidity of the indoor air) has been used by many researchers. Some BES tools such as EnergyPlus (EnergyPlus, 2005) and

TRNSYS use such models in order to take into account the hygroscopic behaviour of the building envelope. The capabilities of this model in terms of modelling indoor humidity changes have been investigated in the past (Janssens & De Paepe, 2005; Steeman et al., 2009). The following section provides a brief description of the EMPD model and its implementation carried out in the ESP-r source code.

EMPD model

This model assumes that only a thin layer of the innermost building material is in interaction with indoor air. The moisture content of this layer is assumed to be constant and uniform. The thickness of this layer can be obtained by the following expression:

$$d = \sqrt{\frac{\delta P_{\text{sat}} \tau}{\rho_{\text{mat}} \xi \pi}} \quad (3)$$

In ESP-r, this thickness for each innermost layer should be provided as input, in the last line of the construction file (*.con) of the model. Figure 1 depicts the flowchart of the implemented EMPD model. As can be seen from this figure, the sorption isotherm of the material should be provided. After initialization, the water content in the layer covered by the penetration depth is calculated. Humidity ratio at saturation can be calculated by (Kerestecioglu et al., 1990):

$$x_{\text{sat},i} = \frac{1}{R_v \rho_a T_{s,i}} e^{\left(\frac{23.7023 - 4111}{T_{s,i} - 35.45} \right)} \quad (4)$$

Then this value is multiplied by the relative humidity to obtain the surface humidity ratio. The construction flux can then be calculated by the summation of all convection fluxes to the indoor environment.

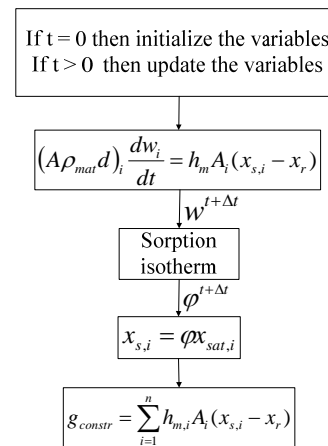


Figure 1 EMPD flowchart

Figure 2 illustrates how EMPD model is integrated in ESP-r. h_c values are calculated by the existing empirical correlations available in ESP-r. Then Lewis analogy is used in order to determine h_m values. Loose coupling is applied, so at each time-step the

EMPD mshakeodel calculates the construction moisture flux and passes it to ESP-r to be included in the moisture balance equation explained in previous section.

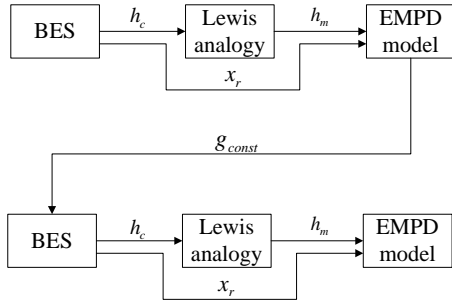


Figure 2 Integration of EMPD model in ESP-r

EXTERNAL COUPLING BETWEEN BES-CFD

BES can provide more realistic boundary conditions than CFD, while CFD can provide higher resolution modelling of flow patterns within air volumes and convective heat and moisture transfer coefficients than BES. A new external coupling prototype is developed for performing the co-simulation between BES (ESP-r) and CFD (FLUENT). The new parts developed in ESP-r source code for the external coupling still are not present in the general release of ESP-r but they will be available in the near future.

In the following sections the features of the prototype such as the coupling requirement, the coupling strategy, the variables and the coupling mechanism are explained.

Coupling requirement

Considering the prevailing range of indoor airflow regimes in the indoor environment, transfer coefficients (h_c and h_m) are influenced by the building envelope state such as interior surface temperature and humidity ratio. Therefore, the coupled solution should be considered for h_c and h_m .

Coupling strategy

The features of existing strategies for BES-CFD coupling such as loose coupling have been discussed in (Zhai et al., 2001; Djunaedy, 2005). For the prototype developed in the present study, a loose coupling strategy has been applied. In this strategy, two or more sets of equations are solved separately and exchange data at each predefined or calculated time step with a specified frequency. There is no iteration process between the two programs to get an agreement on the values at each time step. The loose coupling strategy implemented in this prototype is slightly different from that investigated before (Zhai et al., 2001; Djunaedy, 2005). Figure 3 shows a schematic view of the new coupling strategy applied in the prototype. It allows to call CFD every K time steps.

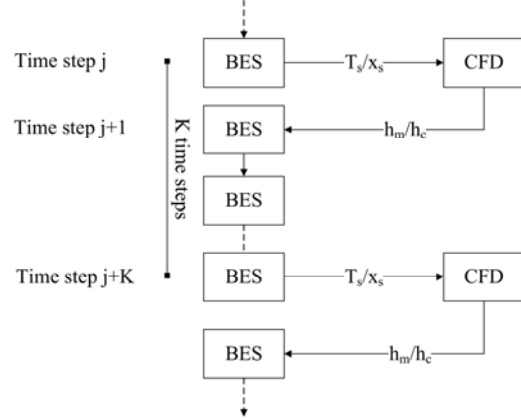


Figure 3 Loose coupling strategy performed at every K time steps of BES

The number K can be set by the user and can vary from 1 to n (n is the total number of time steps in the simulation). For situations in which the boundary conditions do not change rapidly with time, it might not be necessary to call CFD at each BES time-step. In order to avoid similar CFD simulations in case of similar boundary conditions, the user might prefer to call CFD at a different rhythm than every time step in BES.

Coupling variables

Coupling variables are exchanged at the interface of building envelope and the interior domain. BES calculates internal surface temperatures and surface humidity ratios of the zone and passes them to CFD at each time step (assuming K=1 in Figure 3). Then the calculated h_c and h_m values from the converged CFD solution are passed to BES for the next time step. The values of h_c and h_m will be used to calculate the convective heat/moisture transfer to be included in heat/moisture balance equation in BES. The principles of BES-CFD coupling for heat transfer and how h_c for each surface should be treated before being passed to BES have been investigated by (Zhai et al., 2001) and the same procedure has been applied in the coupling procedure in the present study.

In this study however, h_m values as well as h_c values are calculated by the help of user defined functions (UDF) in FLUENT. At any arbitrary points in the concentration boundary layer, mass transfer is due to both fluid bulk motion and diffusion (Incropera & DeWitt, 2002). At the surface of the walls ($y=0$) the transfer is by diffusion only and can be expressed as:

$$g' = -\delta \left. \frac{\partial p_v}{\partial y} \right|_{y=0} \quad (4)$$

Combination of equation 4 and the expression $g' = h_m(p_{v,s} - p_{ref})$ yields

$$h_m = -\delta \left(\left. \frac{\partial p_v}{\partial y} \right|_{y=0} \right) / (p_{v,s} - p_{ref}) \quad (5)$$

The reference vapour pressure in this study is chosen to be the average vapour pressure in the room.

Coupling mechanism

The previous coupling mechanism which was handling the data exchange between ESP-r and FLUENT has been successfully validated by inter-model comparison between a conjugate heat transfer model and BES-CFD model (Mirsadeghi et al., 2008). Based on this validation, an expanded coupling mechanism has been developed for the data exchange between ESP-r and FLUENT.

External data exchange occurs between ESP-r and FLUENT via text file I/O. ESP-r dumps the surface temperatures and humidity ratios into a file. A UNIX script called “format controller” which is based on previous work (Djunaedy, 2005) was developed in order to convert the dumped file into a readable format for FLUENT. Then the format controller calls FLUENT and waits until surface transfer coefficients are calculated. Afterwards, the file that contains the transfer coefficients will be altered into a suitable format by the format controller to be used in ESP-r. This procedure is repeated at each time step in BES in which CFD is called.

CASE STUDY

In this section, the result of introducing the EMPD model in ESP-r and the capabilities of the new prototype are demonstrated by means of an example.

EMPD results

A single zone model was used to investigate the effect of EMPD model on ESP-r results. The model consists of a single room with dimensions of 6 (m) × 8 (m) × 2.7 (m). The internal loads, operation, construction and other configurations except the control strategy (it is explained in the next paragraph) are based on the BESTEST settings (Judkoff & Neymark, 1995).

Initially, the model was simulated for the period of June 28th – July 3rd using the ESP-r standard approach for calculating the air node relative humidity (i.e. using Eq. (1) without considering g_{constr}). Then three separate simulations were performed for the same period considering three different penetration depths for the innermost material layer. In these simulations, a “free floating” simulation was performed to show the effect of moisture buffering on relative humidity of the air node. In these simulations, a “free floating” simulation was performed to show the effect of moisture buffering on relative humidity of the air node. By means of free floating control strategy ESP-r allows the zone temperature to reach whatever the temperature is consistent with the heat gains and losses in the zone. Figure 4 shows the relative humidity of the air node during the simulation period as calculated by ESP-r. In this figure, $d = 0$ mm corresponds to the ESP-r standard calculation and it means that the relative humidity was calculated without considering the hygroscopic effect of the material.

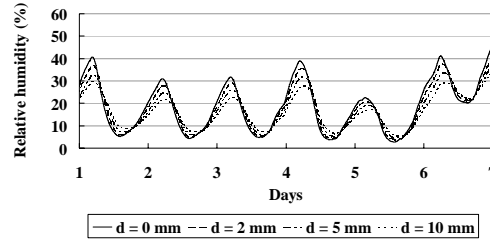


Figure 4 Air node relative humidity

As can be seen from Figure 4, the larger the penetration depth, the more the relative humidity fluctuations of the air node is damped.

Prototype results

The same BESTEST model as in the previous section is used, apart from the climate file that was changed from Denver to Brussels. This climate file was chosen because the future work relates to mold growth analysis and since higher level of humidity exists in Brussels in comparison with Denver, hence there is more risk of mold growth in such a climate. A BES stand-alone simulation for an entire year shows that the indoor relative humidity reaches a maximum on 27th of June. Therefore, this period was chosen to be simulated using the prototype. The prototype needs two separate models for the simulation, which are geometrically identical (a single zone model for BES and a computational grid for CFD). The following sections describe the characteristics of each model in BES and CFD.

- BES model

A snapshot of the model in the ESP-r graphic interface is shown in Figure 5. In the coupled simulation CFD is called every hour to solve the airflow and send the h_c and h_m values to ESP-r.

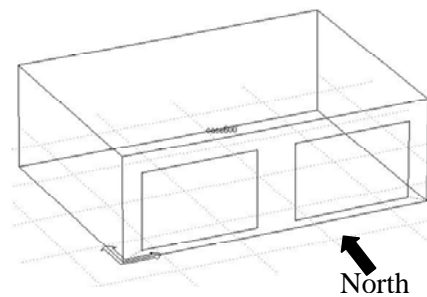


Figure 5 BESTEST geometry in ESP-r graphic interface

- FLUENT model

The room is discretized using a non-uniform structured hexahedral grid (Figure 6). For the CFD simulations the following settings are considered. The $k-\omega$ model is chosen for modelling the turbulence and low-Reynolds modelling is employed for near wall treatment.

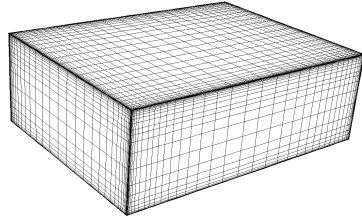


Figure 6 3D computational grid for BES-CFD coupling

Vapour transport modelling is performed by “species transport” available in FLUENT. The density of the humid air is determined using the incompressible ideal gas law. The second order upwind discretization scheme is used and the SIMPLE algorithm is chosen for pressure-velocity coupling. The residuals and the y^+ values were monitored and checked. The existing guidelines for simulating natural convection flows in FLUENT have been used in order to reach an acceptable level of convergence in the simulations (FLUENT 6.3, 2006). In FLUENT, we first perform a steady-state simulation with a one-order-lower Rayleigh number and then a transient simulation with the real Rayleigh number. In the transient simulation, the sensitivity of the h_c and h_m values to the number of iterations per time-step have been investigated in order to obtain the minimum computational time, which resulted in 5 iterations per time-step and the time-step size is 2 seconds.

- Results and discussion

Figure 7 compares the variation of the relative humidity of the air node using ESP-r and using the prototype. As can be seen, the relative humidity calculated by the prototype before 6 h and after 12 h is less than the predicted values by ESP-r stand-alone. Between 6 h and 12 h, the relative humidity predicted by the prototype is higher than that of ESP-r. The maximum difference between these two curves occurs around 10 o'clock and it is equal to 6.5 (%). In order to analyze the differences between these two curves, it is necessary to investigate the variation of h_m values for each surface of the room.

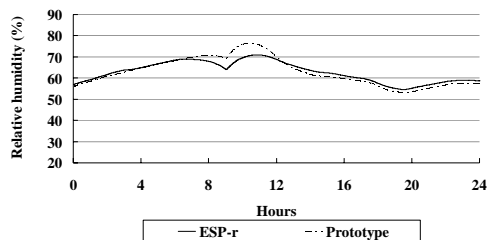


Figure 7 predicted relative humidity of the air node

Figure 8 shows the typical calculated h_m values for the floor and the west wall of the model using the Lewis analogy in ESP-r and CFD in the prototype. h_m values in CFD are averaged over the surface by

means of UDFs. This figure clearly indicates that the h_m values calculated by CFD are most of the time larger than the analogy values. The average h_m values predicted by CFD for the floor and the west wall are respectively 520 % and 292 % larger than the average value calculated by analogy. The underestimation of h_m values by the analogy have been observed in the literature. Differences up to 300% have been reported in the experimental study performed by Derome (1999).

For other surfaces in the room, the predicted h_m values are also always higher than the analogy values. Higher h_m values lead to higher adsorption and desorption of water vapour and therefore influence the relative humidity to be sometimes higher and sometimes lower when calculated with the prototype as shown in Figure 7.

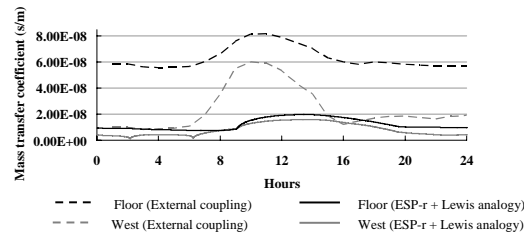


Figure 8 Predicted moisture transfer coefficients for floor and west wall

According to Figure 8, h_m values calculated for the floor by CFD are higher than those of the west wall. It can be explained by the fact that h_m values depend strongly on the flow field of the room. The surface temperature of the windows and the south wall are lower than the surface temperature of the floor and the roof. A downward air circulation dominates the airflow pattern in the room which leads to higher velocities near the surface of the floor when compared to the west and the east wall. Figure 9 demonstrates the contours of velocity magnitude at 11 o'clock close (3 cm) to the floor. Higher velocities can be observed when compared to the contours of velocity close (3 cm) to the west wall (Figure 10) which leads to higher h_m values for the floor.

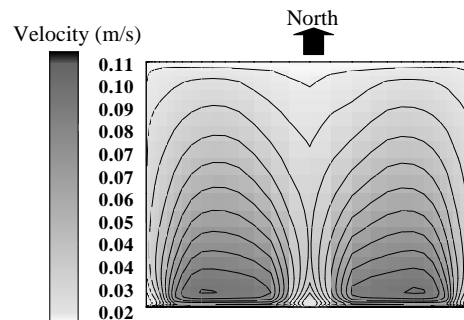


Figure 9 Contours of velocity close to the floor surface

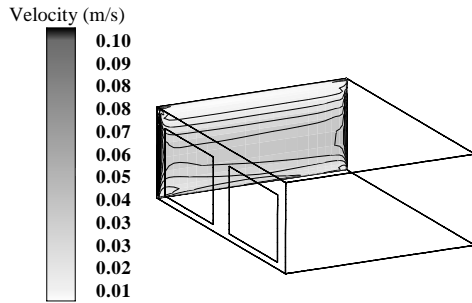


Figure 10 Contours of velocity close to the west wall

Figure 11 illustrates the contours of humidity ratio close to the surface of the west wall (3 cm away from the surface). In reality, 3D heat transfer occurs in the building envelope while 1D heat transfer equation is solved in ESP-r. Similarly, the 3D moisture transfer phenomenon in the building envelope is being represented by a simple moisture inertia model (EMPD model). Consequently, uniform surface temperatures and humidity ratios are sent to CFD for calculation of the airflow. In other words, the distribution of surface temperatures and surface humidity ratios is not considered in the CFD simulation which is an important issue for studying certain performance indicators such as condensation and mold growth in buildings. One possible alternative to overcome this limitation is the use of a conjugate heat and mass transfer models. The conjugate heat and mass transfer model performs the coupled simulation of solid and fluid domain completely within CFD. Due to differences in time scale of fluid and solid domain, this approach is computationally expensive and the difficulties in reaching a converged solution as been reported in the past (Chen et al. 1995). Furthermore, as it was mentioned before the implementation of meteorological boundary conditions and the capabilities for efficient transient modelling are significantly less advanced than in BES tools. A second possible solution is further surface discretization in ESP-r which leads to higher spatial resolution over the surfaces of the room. The differences observed between h_c predictions by a conjugate heat transfer model and the prototype indicates the need for further surface discretization (Mirsadeghi et al., 2008). This approach will be one of the topics for future work.

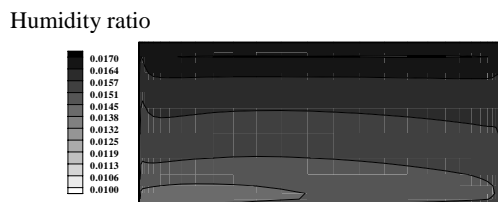


Figure 11 Humidity ratio close to the west wall

CONCLUSIONS

An external coupling procedure between ESP-r and FLUENT (prototype) was developed which includes heat, air and moisture as the physical domains. For this purpose, a simplified moisture inertia model was first implemented within ESP-r. Then the airflow pattern and distribution of temperature and mass fraction of water vapour in a single zone model were investigated using the prototype. The results of ESP-r stand-alone were compared to the results of the prototype.

The following conclusions can be drawn:

- The relative humidity calculation for the air node using different tools (ESP-r and the prototype) resulted in some differences. For this simple geometry, the difference could be as high as 6.5 (%) for some hours of the day if CFD is involved in the simulation. For complex geometries, this difference might be more remarkable, highlighting the impact of coupling CFD with BES.
- Using the prototype has resulted in much higher convective moisture transfer coefficients when compared to the values predicted by ESP-r which is using Lewis analogy for this case. Such large differences have been reported in the past between the experiments and the analogy. Hence affecting the adsorption and desorption rate which resulted in the differences in relative humidity calculation.
- Surface discretization in BES tools could potentially allow higher spatial resolution at the boundaries when coupled with CFD tools. This might result in better prediction of some performance indicators such as condensation and mold growth.

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NOMENCLATURE

A	Heat and moisture transfer surface area (m^2)
d	Penetration depth (m)
g	Moisture gain (kg/s)
g'	Moisture flux (kg/sm^2)
h_m	Convective moisture transfer coefficient (s/m)
h_c	Convective heat transfer coefficient (W/m^2K)
p	Water vapour pressure (Pa)
R_v	Gas constant for water vapour (J/kgK)

T	Temperature (K)
t	Time (s)
V	Volume of the zone (m^3)
w	Water content (kg/kg)
x	Humidity ratio (kg/kg)
y	Position axis perpendicular to the surface
y^+	Mesh-dependent dimensionless distance
δ	Water vapour permeability (kg/msPa)
ξ	Hygroscopic moisture capacity (kg/ m^3)
ρ	Density (kg/ m^3)
τ	Period of indoor humidity variations (s)
ϕ	Relative humidity (%)

Subscripts, superscripts and indices

<i>equ</i>	Equipment
<i>peo</i>	People
<i>ven</i>	Ventilation
<i>inf</i>	Infiltration
<i>sys</i>	System (HVAC)
<i>constr</i>	Construction
<i>ref</i>	Reference
<i>mat</i>	Material
<i>a</i>	Air
<i>i</i>	Summation index over zone surfaces
<i>r</i>	Zone air node
<i>s</i>	Surface condition
<i>v</i>	Vapour

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